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      5 NOV 30 PHAR reloaded with additional data
NEWS
         DEC 01 LISA now available on STN
NEWS
      6
      7
         DEC 09
                 12 databases to be removed from STN on December 31, 2004
NEWS
         DEC 15
                 MEDLINE update schedule for December 2004
NEWS
      R
NEWS 9 DEC 17 ELCOM reloaded; updating to resume; current-awareness
                 alerts (SDIs) affected
NEWS 10 DEC 17 COMPUAB reloaded; updating to resume; current-awareness
                 alerts (SDIs) affected
                 SOLIDSTATE reloaded; updating to resume; current-awareness
NEWS
     11 DEC 17
                 alerts (SDIs) affected
     12 DEC 17 CERAB reloaded; updating to resume; current-awareness
 NEWS
                 alerts (SDIs) affected
                 THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
 NEWS 13 DEC 17
 NEWS 14 DEC 30 EPFULL: New patent full text database to be available on STN
 NEWS 15 DEC 30 CAPLUS - PATENT COVERAGE EXPANDED
 NEWS 16 JAN 03 No connect-hour charges in EPFULL during January and
                 February 2005
     17 FEB 25
                 CA/CAPLUS - Russian Agency for Patents and Trademarks
 NEWS
                  (ROSPATENT) added to list of core patent offices covered
                 STN Patent Forums to be held in March 2005
     18 FEB 10
 NEWS
                 STN User Update to be held in conjunction with the 229th ACS
 NEWS 19 FEB 16
                 National Meeting on March 13, 2005
 NEWS 20 FEB 28
                 PATDPAFULL - New display fields provide for legal status
                 data from INPADOC
 NEWS 21 FEB 28 BABS - Current-awareness alerts (SDIs) available
 NEWS 22 FEB 28 MEDLINE/LMEDLINE reloaded
 NEWS 23 MAR 02 GBFULL: New full-text patent database on STN
 NEWS 24 MAR 03 REGISTRY/ZREGISTRY - Sequence annotations enhanced
 NEWS 25 MAR 03 MEDLINE file segment of TOXCENTER reloaded
 NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
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FILE 'HOME' ENTERED AT 14:45:11 ON 18 MAR 2005

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.63 0.63

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 14:47:12 ON 18 MAR 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 17 MAR 2005 HIGHEST RN 845858-62-0 DICTIONARY FILE UPDATES: 17 MAR 2005 HIGHEST RN 845858-62-0

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> Uploading C:\Program Files\Stnexp\Queries\10677288c.str

## L1 STRUCTURE UPLOADED

=> s l1 STRUCTURE TOO LARGE - SEARCH ENDED A structure in your query is too large. You may delete attributes or atoms to reduce the size of the structure and try again.

=>
Uploading C:\Program Files\Stnexp\Queries\10677288e.str

#### L2 STRUCTURE UPLOADED

=> s 12 STRUCTURE TOO LARGE - SEARCH ENDED A structure in your query is too large. You may delete attributes or atoms to reduce the size of the structure and try again.

=>

Uploading C:\Program Files\Stnexp\Queries\10677288f.str

L3 STRUCTURE UPLOADED

=> s 13

SAMPLE SEARCH INITIATED 14:52:17 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2763 TO ITERATE

36.2% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 52108 TO 58412 PROJECTED ANSWERS: 1 TO 154

L4 1 SEA SSS SAM L3

=> search 13
ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.
ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:full
FULL SEARCH INITIATED 14:52:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 56351 TO ITERATE

100.0% PROCESSED 56351 ITERATIONS SEARCH TIME: 00.00.01

47 ANSWERS

1 ANSWERS

L5 47 SEA SSS FUL L3

=>

Uploading C:\Program Files\Stnexp\Queries\10677288g.str

L6 STRUCTURE UPLOADED

=> s 16

STRUCTURE TOO LARGE - SEARCH ENDED
A structure in your query is too large. You may delete attributes or atoms to reduce the size of the structure and try again.

Uploading C:\Program Files\Stnexp\Queries\10677288h.str

L7 STRUCTURE UPLOADED

=> s 17

STRUCTURE TOO LARGE - SEARCH ENDED
A structure in your query is too large. You may delete attributes or atoms to reduce the size of the structure and try again.

=>
Uploading C:\Program Files\Stnexp\Queries\10677288i.str

L8 STRUCTURE UPLOADED

=> s 18

STRUCTURE TOO LARGE - SEARCH ENDED
A structure in your query is too large. You may delete attributes or atoms to reduce the size of the structure and try again.

=>

Uploading C:\Program Files\Stnexp\Queries\10677288j.str

## L9 STRUCTURE UPLOADED

=> s 19

STRUCTURE TOO LARGE - SEARCH ENDED
A structure in your query is too large. You may delete attributes or atoms to reduce the size of the structure and try again.

=>

Uploading C:\Program Files\Stnexp\Queries\10677288k.str

L10 STRUCTURE UPLOADED

=> d 110

L10 HAS NO ANSWERS

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s 110

STRUCTURE TOO LARGE - SEARCH ENDED A structure in your query is too large. You may delete attributes or atoms to reduce the size of the structure and try again.

=>

Uploading C:\Program Files\Stnexp\Queries\106772881.str

L11 STRUCTURE UPLOADED

=> s 111

SAMPLE SEARCH INITIATED 15:08:25 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 1859 TO ITERATE

53.8% PROCESSED 1000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*
PROJECTED ITERATIONS: 34594 TO 39766
PROJECTED ANSWERS: 1 TO 118

L12 1 SEA SSS SAM L11

=> search 111

ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:.

Page 4

1 ANSWERS

ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET: full FULL SEARCH INITIATED 15:08:33 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 38377 TO ITERATE

100.0% PROCESSED 38377 ITERATIONS

15 ANSWERS

SEARCH TIME: 00.00.01

L13 15 SEA SSS FUL L11

=> d his

(FILE 'HOME' ENTERED AT 14:45:11 ON 18 MAR 2005)

FILE 'REGISTRY' ENTERED AT 14:47:12 ON 18 MAR 2005
L1 STRUCTURE UPLOADED

L2 STRUCTURE UPLOADED
L3 STRUCTURE UPLOADED

L4 1 S L3

L5 47 SEARCH L3 FULL
L6 STRUCTURE UPLOADED
L7 STRUCTURE UPLOADED
L8 STRUCTURE UPLOADED
L9 STRUCTURE UPLOADED

L10 STRUCTURE UPLOADED L11 STRUCTURE UPLOADED

L12 1 S L11

L13 15 SEARCH L11 FULL

=> s 15 or 113

L14 47 L5 OR L13

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 337.28 337.91

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=> s 114

# => d 115 fbib ab hitstr 1-13

L15 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:861007 CAPLUS

DN 142:32437

TI N1-Substituent Effects in the Selective Delivery of Polyamine Conjugates into Cells Containing Active Polyamine Transporters

AU Gardner, Richard Andrew; Delcros, Jean-Guy; Konate, Fanta; Breitbeil, Fred, III; Martin, Benedicte; Sigman, Michael; Huang, Min; Phanstiel, Otto, IV

CS Department of Chemistry, University of Central Florida, Orlando, FL, 32816-2366, USA

SO Journal of Medicinal Chemistry (2004), 47(24), 6055-6069 CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

Several N1-arylalkylpolyamines containing various aromatic ring systems were AB synthesized as their resp. HCl salts. The N1-substituents evaluated ranged in size from N1-benzyl, N1-naphthalen-1-ylmethyl, N1-2-(naphthalen-1-yl)ethyl, N1-3-(naphthalen-1-yl)propyl, N1anthracen-9-ylmethyl, N1-2-(anthracen-9-yl)ethyl, N1-3-(anthracen-9yl)propyl, and pyren-1-ylmethyl. The polyamine architecture was also altered and ranged from diamine to triamine and tetraamine systems. Biol. activities in L1210 (murine leukemia), Chinese hamster ovary (CHO), and CHO's polyamine transport-deficient mutant (CHO-MG) cell lines were investigated via IC50 cytotoxicity detns. Ki values for spermidine uptake were also determined in L1210 cells. The size of the N1-arylalkyl substituent as well as the polyamine sequence used had direct bearing on the observed cytotoxicity profiles. N1-Tethers longer than ethylene showed dramatic loss of selectivity for the polyamine transporter (PAT) as shown in a CHO/CHO-MG cytotoxicity screen. In summary, there are clear limits to the size of N1-substituents, which can be accommodated by the polyamine transporter. A direct correlation was observed between polyamine-conjugate uptake and cytotoxicity. In this regard, a cytotoxicity model was proposed, which describes a hydrophobic pocket of set dimensions adjacent to the putative PAT polyamine-binding site.

## IT 805229-80-5P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(N1-substituent effects in selective delivery of polyamine conjugates into cells containing active polyamine transporters)

RN 805229-80-5 CAPLUS

CN 1,4-Butanediamine, N-(4-aminobutyl)-N'-[2-(2-naphthalenyl)ethyl]-, trihydrochloride (9CI) (CA INDEX NAME)

●3 HCl

## IT 805229-79-2

RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(N1-substituent effects in selective delivery of polyamine conjugates into cells containing active polyamine transporters)

RN 805229-79-2 CAPLUS

CN 1,4-Butanediamine, N-(4-aminobutyl)-N'-(4-pyrenylmethyl)-, trihydrochloride (9CI) (CA INDEX NAME)

## ●3 HCl

# RE.CNT 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:606913 CAPLUS

DN 141:310543

- TI Self-organization of oligomeric helical stacks controlled by substrate binding in a tobacco mosaic virus like self-assembly process
- AU Petitjean, Anne; Nierengarten, Helene; van Dorosselaer, Alain; Lehn, Jean-Marie
- CS Laboratoire de Chimie Supramoleculaire, ISIS, Strasbourg, BP 70028, Fr.
- SO Angewandte Chemie, International Edition (2004), 43(28), 3695-3699 CODEN: ACIEF5; ISSN: 1433-7851
- PB Wiley-VCH Verlag GmbH & Co. KGaA
- DT Journal
- LA English
- AB Self-assembly with a twist: Linear polyammonium threads are templates in the organization of helical heterocyclic building blocks to form stacks of helixes as a model for the Tobacco Mosaic Virus. The length of the cationic substrate and the spacing of the pos. charges within the thread dictate the size of the final self-organized supramol. architecture.
- IT 176977-11-0 767330-07-4 767330-09-6
  RL: BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); BIOL (Biological study); PROC

(Process)
 (modeling of tobacco mosaic virus self-assembly through
 self-organization of oligomeric helical stacks of organic compds.)

RN 176977-11-0 CAPLUS

CN 1,2-Ethanediamine, N-(2-naphthalenylmethyl)-N'-[2-[(2-naphthalenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 767330-07-4 CAPLUS

CN 1,3-Propanediamine, N-(2-naphthalenylmethyl)-N'-[3-[(2-naphthalenylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)

RN 767330-09-6 CAPLUS

CN 1,4-Butanediamine, N,N'-bis[3-[(2-naphthalenylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:827041 CAPLUS

DN 140:35486

TI Defining the Molecular Requirements for the Selective Delivery of `Polyamine Conjugates into Cells Containing Active Polyamine Transporters

AU Wang, Chaojie; Delcros, Jean-Guy; Cannon, Laura; Konate, Fanta; Carias, Horacio; Biggerstaff, John; Gardner, Richard Andrew; Phanstiel, Otto

CS Groupe de Recherche en Therapeutique Anticancereuse, Faculte de Medecine, University of Rennes 1, Rennes, 35043, Fr.

SO Journal of Medicinal Chemistry (2003), 46(24), 5129-5138 CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

AB Several N1-substituted polyamines containing various spacer units between nitrogen centers were synthesized as their resp. HCl salts. The N1-substituents included benzyl, naphthalen-1-ylmethyl, anthracen-9-ylmethyl, and pyren-1-ylmethyl. The polyamine spacer units ranged from generic (4,4-triamine, 4,3-triamine, and diaminooctane) spacers to more exotic [2-(ethoxy)ethanoxy-containing diamine, hydroxylated 4,3-triamine, and cyclohexylene-containing triamine] spacers. Two control compds. were also evaluated:N-(anthracen-9-ylmethyl)-butylamine and N-(anthracen-9-ylmethyl)-butanediamine. Biol. activities in L1210 (murine

leukemia),  $\alpha$ -difluoromethylornithine (DFMO)-treated L1210, and Chinese hamster ovary (CHO) and its polyamine transport-deficient mutant (CHO-MG) cell lines were investigated via IC50 cytotoxicity detns. Ki values for spermidine uptake were also determined in L1210 cells. Of the series studied, the N1-benzyl-4,4-triamine derivative (6) had significantly higher IC50 values (lower cytotoxicity) in the L1210, CHO, and CHO-MG cell lines. A cellular debenzylation process was observed in L1210 cells with 6 and generated "free" homospermidine. The size of the N1-arylmethyl substituent had direct bearing on the observed cytotoxicity in CHO-MG cells. The N1-naphthalenylmethyl, N1-anthracenylmethyl, and N1-pyrenylmethyl 4,4-triamines had similar toxicity (IC50s: .apprx.0.5 μM) in CHO cells, which have an active polyamine transporter (PAT). However, this series had IC50 values of >100  $\mu$ M, 66.7  $\mu$ M, and 15.5  $\mu$ M, resp., in CHO-MG cells, which are PAT-deficient. The observed lower cytotoxicity in the PAT-deficient CHO-MG cell line supported the premise that the conjugates use PAT for cellular entry. In general, moderate affinities for the polyamine transporter were observed for the N-arylmethyl 4,4-triamine series with their L1210 Ki values all near 3 μM. In summary, the 4,4-triamine motif was shown to facilitate entry of polyamine conjugates into cells containing active polyamine transporters.

IT 635304-07-3P

RN

CN

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(defining the mol. requirements for selective delivery of polyamine conjugates into cells containing active polyamine transporters)
635304-07-3 CAPLUS

1,4-Butanediamine, N-(4-aminobutyl)-N'-(1-pyrenylmethyl)-, trihydrochloride (9CI) (CA INDEX NAME)

$$CH_2-NH-(CH_2)_4-NH-(CH_2)_4-NH_2$$

# •3 HCl

RE.CNT 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:477826 CAPLUS

DN 137:262736

TI Open-chain polyazaalkanes functionalised with pyrene groups as sensing fluorogenic receptors for metal ions

AU Sancenon, Felix; Descalzo, Ana Belen; Lloris, Jose Manuel; Martinez-Manez, Ramon; Pardo, Teresa; Segui, Maria Jesus; Soto, Juan

CS Departamento de Quimica, Universidad Politecnica de Valencia, Valencia, 46071, Spain

SO Polyhedron (2002), 21(14-15), 1397-1404 CODEN: PLYHDE; ISSN: 0277-5387

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 137:262736

The new open-chain polyazaalkanes ligands (I; R = H, CH2-pyrenyl, AB CH2CH2NH2, CH2CH2NH-pyrenyl, L1-L4) functionalized with one or two pyrene groups were synthesized and characterized and their potential use as selective cation and anion sensing chemosensors studied. Solution studies by potentiometric methods were carried out in the presence of Cu2+ and Zn2+ in MeCN-H2O (70:30 volume/volume, 0.1 mol dm-3 Bu4NClO4, 25°) and the results are compared with those reported for the analogous nonfunctionalized ligand triethylentetraamine (tta). The fluorescence behavior of the ligands L1-L4 was studied as a function of the pH in the presence of the metal cations Ni2+, Cu2+, Zn2+, Cd2+, Hg2+ and Pb2+ in MeCN-H2O 70:30 volume/volume mixts. The Zn2+ and Cd2+ cations enhance the fluorescence emission of the L1-L4 chemosensors at basic pH, whereas Cu2+ induce quenching of the fluorescence emission at acid pH. The fluorescence behavior of L1-L4 receptors was also studied as a function of the pH in MeCN-H2O 70:30 volume/volume in the presence of anions.

IT 461668-36-0P 461668-37-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and fluorescence with and without transition metal ions)

RN 461668-36-0 CAPLUS

CN 1,2-Ethanediamine, N-[2-[(2-aminoethyl)amino]ethyl]-N'-[2-[(1-pyrenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

— CH2- CH2- NH2

RN 461668-37-1 CAPLUS

CN 1,2-Ethanediamine, N-[2-[(1-pyrenylmethyl)amino]ethyl]-N'-[2-[[2-[(1-pyrenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

IT 461668-30-4P 461668-31-5P 461668-32-6P

461668-33-7P

RN 461668-30-4 CAPLUS

CN 1,2-Ethanediamine, N-(2-aminoethyl)-N'-[2-[(1-pyrenylmethyl)amino]ethyl]-, tetrahydrochloride (9CI) (CA INDEX NAME)

$$CH_2-NH-CH_2-CH_2-NH-CH_2-CH_2-NH-CH_2-CH_2-NH_2$$

## •4 HCl

RN 461668-31-5 CAPLUS

CN 1,2-Ethanediamine, N,N'-bis[2-[(1-pyrenylmethyl)amino]ethyl]-, tetrahydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

## • 4 HCl

PAGE 1-B

RN 461668-32-6 CAPLUS

CN 1,2-Ethanediamine, N-[2-[(2-aminoethyl)amino]ethyl]-N'-[2-[(1-pyrenylmethyl)amino]ethyl]-, pentahydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

● 5 HCl

PAGE 1-B

- CH<sub>2</sub>- CH<sub>2</sub>- NH<sub>2</sub>

RN 461668-33-7 CAPLUS

CN 1,2-Ethanediamine, N-[2-[(1-pyrenylmethyl)amino]ethyl]-N'-[2-[[2-[(1-pyrenylmethyl)amino]ethyl]amino]ethyl]-, pentahydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

● 5 HCl

PAGE 1-B

IT 461668-34-8P 461668-35-9P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, protonation, fluorescence and complexation with copper(II) and zinc)

RN 461668-34-8 CAPLUS

CN 1,2-Ethanediamine, N-(2-aminoethyl)-N'-[2-[(1-pyrenylmethyl)amino]ethyl]-(9CI) (CA INDEX NAME)

RN 461668-35-9 CAPLUS

CN 1,2-Ethanediamine, N,N'-bis[2-[(1-pyrenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

IT 461668-34-8D, copper complex 461668-35-9D, copper and

zinc complexes

RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(stability constant)

RN 461668-34-8 CAPLUS

CN 1,2-Ethanediamine, N-(2-aminoethyl)-N'-[2-[(1-pyrenylmethyl)amino]ethyl](9CI) (CA INDEX NAME)

$$\begin{picture}(20,10) \put(0,0){\line(1,0){10}} \put(0,$$

RN 461668-35-9 CAPLUS

CN 1,2-Ethanediamine, N,N'-bis[2-[(1-pyrenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-B

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:319661 CAPLUS

DN 134:336203

TI Substituted succinic acid metallo- $\beta$ -lactamase inhibitors, their preparation, and their use in treating bacterial infections

IN Balkovec, James M.; Greenlee, Mark L.; Olson, Steven H.; Rouen, Gregory P.

PA Merck & Co., Inc., USA

SO PCT Int. Appl., 129 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1																			
										APPLICATION NO.									
ΡI	WO						A1 20010503			WO 2000-US29707									
		W: AE, AG, AL,																	
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												KZ,							
			LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	
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	EP	1227721		A1 20020807				EP 2	-000	9754	54		2	0001	027				
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			US 1999-162370P	P	19991028
			WO 2000-US29707	W	20001027
AU 771274	B2	20040318	AU 2001-13504		20001027
			US 1999-162370P	P	19991028
			WO 2000-US29707	W	20001027
US 2003078418	A1	20030424	US 2002-99790		20020315
			US 1999-162370P	P	19991028
			US 2000-697415	A3	20001026
US 2003207859	A1	20031106	US 2003-339043		20030109
		•	US 1999-162370P	P	19991028
			US 2000-697415	A3	20001026

OS MARPAT 134:336203

Substituted succinic acid metallo- $\beta$ -lactamase inhibitors are provided which are useful potentiators of  $\beta$ -lactam antibiotics. Accordingly, the invention provides a method of treating bacterial infections in animals or humans which comprises administering, together with a  $\beta$ -lactam antibiotic, a therapeutically effective amount of a succinic acid derivative of the invention, or a pharmaceutically acceptable salt, prodrug, anhydride, or solvate thereof.

IT 337907-35-4

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(succinic acid derivative metallo- $\beta$ -lactamase inhibitors, preparation, and use in treating bacterial infections)

RN 337907-35-4 CAPLUS

CN 2-Naphthalenepropanaminium, N-[3-[(3-aminopropyl)amino]propyl]-6-[(2S,3S)-2,3-dicarboxy-4-phenylbutyl]-N,N-dimethyl-, chloride, dihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$H_{2N}$$
 (CH<sub>2</sub>)  $\frac{H}{3}$  (CH<sub>2</sub>)  $\frac{N}{3}$  (C

• c1 -

### ●2 HCl

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1998:34062 CAPLUS

DN 128:188273

TI Polyamine derivatives as inhibitors of trypanothione reductase and assessment of their trypanocidal activities

AU O'sullivan, Mary C.; Zhou, Qibing; Li, Zhili; Durham, Timothy B.; Rattendi, Donna; Lane, Schennella; Bacchi, Cyrus J.

CS Department of Chemistry, Indiana State University, Terre Haute, IN, 47809, USA

SO Bioorganic & Medicinal Chemistry (1997), 5(12), 2145-2155 CODEN: BMECEP; ISSN: 0968-0896

PB Elsevier Science Ltd.

DT Journal

LA English

Trypanothione reductase (TR) occurs exclusively in trypanosomes and AB leishmania, which are the etiol. agents of many diseases. TR plays a vital role in the antioxidant defenses of these parasites and inhibitors of TR have potential as antitrypanosomal agents. We describe the syntheses of several spermine and spermidine derivs. and the inhibiting effects of these compds. on T. cruzi TR. All of the inhibiting compds. displayed competitive inhibition of TR-mediated reduction of trypanothione disulfide. The three most effective compds. studied were N4,N8-bis(3-phenylpropyl)spermine (I), N4,N8-bis(2-naphthylmethyl)spermine (II), and N1,N8-bis(2-naphthylmethyl)spermidine (III), with Ki values of 3.5, 5.5 and 9.5  $\mu M$ , resp. Compds. I, II, and III were found to be potent trypanocides in vitro with IC50 values ranging from 0.19 to 0.83  $\mu M$  against four T. brucei ssp. strains. However, these compds. did not prolong the lives of mice infected with trypanosomes. This work indicates that certain polyamine derivs. which target a unique pathway in Trypanosomatidae have potential as antitrypanosomal agents.

IT 168101-39-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of polyamine derivs. as inhibitors of trypanothione reductase and assessment of their trypanocidal activities)

RN 168101-39-1 CAPLUS

CN 1,4-Butanediamine, N-(2-naphthalenylmethyl)-N'-[3-[(2-naphthalenylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)

$$CH_2-NH-(CH_2)_4-NH-(CH_2)_3-NH-CH_2$$

RE.CNT 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1997:237990 CAPLUS

DN 127:12989

TI Inhibiting effects of spermidine derivatives on Trypanosoma cruzi trypanothione reductase

AU O'Sullivan, Mary C.; Dalrymple, Damon M.; Zhou, Qibing

CS Department Chemistry, Indiana State University, Terre Haute, IN, 47809, USA

SO Journal of Enzyme Inhibition (1996), 11(2), 97-114 CODEN: ENINEG; ISSN: 8755-5093

PB Harwood

DT Journal

LA English

AB The preparation of several spermidine derivs. is described and their inhibition kinetics in the reduction of trypanothione by Trypanosoma cruzi trypanothione reductase (I) were studied. Spermidine derivs. containing hydrophobic aromatic

substituents were found to be competitive inhibitors of I. N4-acylated spermidine derivs. were less effective inhibitors than the corresponding N4-alkylated derivs. The most effective compds. studied were N1,N8-bis(2-naphthylmethyl)spermidine (II) and N4-(2-naphthylmethyl)spermidine, with Ki values of 9.5 and 108  $\mu\text{M}$ , resp. The results of these studies indicated the relative importance of specific structural features required for spermidine derivs. to be inhibitors of I. The most potent compds. in this study contained naphthyl substituents; compds. with benzyl substituents were less effective inhibitors. Spermidine derivs. such as II are easy to prepare and are inexpensive and thus may provide a new direction for the development of affordable antitrypanosomal agents.

IT 168101-39-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of spermidine derivs. and their inhibition kinetics with Trypanosoma cruzi trypanothione reductase)

RN 168101-39-1 CAPLUS

CN 1,4-Butanediamine, N-(2-naphthalenylmethyl)-N'-[3-[(2-naphthalenylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)

L15 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1996:238014 CAPLUS

DN 125:10253

TI Terminal Alkylation of Linear Polyamines

AU Sclafani, Joseph A.; Maranto, Maria T.; Sisk, Thomas M.; Van Arman, Scott A.

CS Department of Chemistry, Franklin and Marshall College, Lancaster, PA, 17604-3003, USA

SO Journal of Organic Chemistry (1996), 61(9), 3221-2 CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

AB Linear polyamines are known to be interesting agents for a wide variety of reasons. Their synthetic elaboration has been limited but is of fundamental importance. The general use of a simple reductive amination sequence for the selective alkylation of terminal amines in linear polyamines is reported. Yields of up to 73% are reported.

IT 176977-06-3P 176977-07-4P 176977-08-5P

176977-11-0P 176977-12-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 176977-06-3 CAPLUS

CN 1,2-Ethanediamine, N-(2-naphthalenylmethyl)-N'-[2-[(2-naphthalenylmethyl)amino]ethyl]-, trihydrochloride (9CI) (CA INDEX NAME)

●3 HCl

RN 176977-07-4 CAPLUS

CN 1,2-Ethanediamine, N,N'-bis[2-[(2-naphthalenylmethyl)amino]ethyl]-, tetrahydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

•4 HCl

PAGE 1-B

RN 176977-08-5 CAPLUS

CN 1,2-Ethanediamine, N-[2-[(2-naphthalenylmethyl)amino]ethyl]-N'-[2-[[2-[(2-naphthalenylmethyl)amino]ethyl]amino]ethyl]-, pentahydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

●5 HCl

RN 176977-11-0 CAPLUS

CN 1,2-Ethanediamine, N-(2-naphthalenylmethyl)-N'-[2-[(2-naphthalenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 176977-12-1 CAPLUS

CN 1,2-Ethanediamine, N-[2-[(2-naphthalenylmethyl)amino]ethyl]-N'-[2-[[2-[(2-naphthalenylmethyl)amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

- L15 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 1995:796292 CAPLUS
- DN 123:221529
- TI Novel polyamine derivatives as potent competitive inhibitors of Trypanosoma cruzi trypanothione reductase
- AU O'Sullivan, Mary C.; Zhou, Qibing
- CS Department of Chemistry, Indiana State University, Terre Haute, IN, 47809,
- SO Bioorganic & Medicinal Chemistry Letters (1995), 5(17), 1957-60 CODEN: BMCLE8; ISSN: 0960-894X
- PB Elsevier
- DT Journal
- LA English
- AB The inhibiting effects of several spermidine and spermine derivs. on T. cruzi trypanothione reductase were assessed. Spermidine and spermine derivs. containing hydrophobic aromatic substituents were competitive inhibitors

of trypanothione reductase. The most effective compds. tested were N1,N8-bis(2-naphthylmethyl)spermidine, N4,N8-bis(2-naphthylmethyl)spermine and N4,N8-bis(3-phenylpropyl)spermine.

IT 168101-39-1

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study) (novel polyamine derivs. as potent competitive inhibitors of Trypanosoma cruzi trypanothione reductase)

RN 168101-39-1 CAPLUS

CN 1,4-Butanediamine, N-(2-naphthalenylmethyl)-N'-[3-[(2-naphthalenylmethyl)amino]propyl]- (9CI) (CA INDEX NAME)

$$CH_2-NH-(CH_2)_4-NH-(CH_2)_3-NH-CH_2$$

L15 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:404656 CAPLUS

DN 123:198340

TI Platelet aggregation inhibiting and anticoagulant effects of oligoamines. XXVIII: Oligoamines with fluorescent properties. Part C: Fluorescent oligoamines with enhanced hydrophilic properties

AU Rehse, Klaus; Seidel, Torsten

CS Institut Pharmazie Freie, Universitaet Berlin, Berlin, 14195, Germany

SO Archiv der Pharmazie (Weinheim, Germany) (1995), 328(2), 131-5. CODEN: ARPMAS; ISSN: 0365-6233

PB VCH

DT Journal

LA English

AB Fifteen fluorescent oligoamines with one or two fluorescent groups and two or three basic N-functions were prepared and tested for antiplatelet activity (Born-test). Five compds. involving three different fluorophores, i.e. 2-fluorenyl, 1-pyrenyl, and 9-phenanthryl, show an IC50 of 7-11 µmol/L. They are suitable to serve as probes in the field of oligoamine-biopolymer interactions. An example compound is N-[4-(9H-fluoren-2-yl)butyl]-N'-octyl-1,5-pentanediamine dihydrochloride.

IT 167562-38-1P 167562-39-2P 167562-40-5P 167562-41-6P 167562-42-7P 167562-43-8P 167562-44-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of oligoamines as anticoagulants and platelet aggregation inhibitors)

RN 167562-38-1 CAPLUS

CN 1,2-Ethanediamine, N-(1-pyrenylmethyl)-N'-[2-[(1-pyrenylmethyl)amino]ethyl]-, trihydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

●3 HCl

PAGE 1-B

CN

RN 167562-39-2 CAPLUS

1,3-Propanediamine, N-(1-pyrenylmethyl)-N'-[2-[(1-pyrenylmethyl)amino]ethyl]-, trihydrochloride (9CI) (CA INDEX NAME)

●3 HCl

RN 167562-40-5 CAPLUS

CN 1,3-Propanediamine, N-(1-pyrenylmethyl)-N'-[3-[(1-pyrenylmethyl)amino]propyl]-, trihydrochloride (9CI) (CA INDEX NAME)

●3 HCl

RN 167562-41-6 CAPLUS

CN 1,4-Butanediamine, N-(1-pyrenylmethyl)-N'-[3-[(1-

pyrenylmethyl)amino]propyl]-, trihydrochloride (9CI) (CA INDEX NAME)

$$CH_2$$
-  $NH$ -  $(CH_2)_4$ -  $NH$ -  $(CH_2)_3$ -  $NH$ -  $CH_2$ 

# ●3 HCl

RN 167562-42-7 CAPLUS

CN 1,3-Propanediamine, N-(9-phenanthrenylmethyl)-N'-[2-[(9-phenanthrenylmethyl)amino]ethyl]-, trihydrochloride (9CI) (CA INDEX NAME)

## ●3 HCl

RN 167562-43-8 CAPLUS

CN 1,3-Propanediamine, N-(9-phenanthrenylmethyl)-N'-[3-[(9-phenanthrenylmethyl)amino]propyl]-, trihydrochloride (9CI) (CA INDEX NAME)

# ●3 HCl

RN 167562-44-9 CAPLUS

CN 1,3-Propanediamine, N-(2-naphthalenylmethyl)-N'-[2-[(2-naphthalenylmethyl)amino]ethyl]-, trihydrochloride (9CI) (CA INDEX NAME)

## ●3 HCl

L15 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1994:457092 CAPLUS

DN 121:57092

TI Nonpeptide Peptidomimetic Antagonists of the Neuropeptide Y Receptor: Benextramine Analogs with Selectivity for the Peripheral Y2 Receptor

AU Chaurasia, Chandra; Misse, Gregory; Tessel, Richard; Doughty, Michael B.

CS Departments of Medicinal Chemistry and Pharmacology and Toxicology, University of Kansas, Lawrence, KS, 66045, USA

SO Journal of Medicinal Chemistry (1994), 37(14), 2242-8 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

- AB A new series of benextramine analogs [RCH2NH(CH2)6XCH2CH2Y]2 [I; R = 2-naphthyl, 1-adamantyl, X = NH, NC(NH2):NH, Y = S, CH2] were prepared as neuropeptide Y (NPY) functional group mimetics and tested for N-[propionyl-3H]NPY ([3]NPY) displacement activity in rat brain membrane homogenates and for NPY receptor antagonist activity in the rat femoral artery. The tetraamine carbon analog I (R = 2-naphthyl, X = NH, Y = CH2) was equipotent with benextramine in a rat brain [3H]NPY displacement assay, suggesting that the disulfide is not a necessary feature of the benextramine activity, although this analog maintained selectivity for the benextramine-sensitive binding site population. Bis(N,N-dialkylguanyl) disulfide and carbon analogs I [R = 2-naphthyl, 1-adamantyl, X =NC(NH2):NH, Y = S, CH2] were 3-4 times more potent than their resp. controls in displacing [3H]NPY from rat brain membrane homogenates, and maintained selectivity for the benextramine-sensitive, Y1 binding site population. However, the activity of the carbon analog I.4HCl [R = 2-naphthyl, X = NC(NH2):NH, Y = CH2] showed a different profile in a femoral artery vasoconstriction assay; at 1.0 nM, this analog shifted the concentration-effect curve of the Y2-selective agonist NPY(13-36) to the right without a significant change in the maximum effect, while even at 1.0 mM it had no effect on the vasoconstrictive activity of the Y1-selective agonist [Leu31, Pro34] - NPY. Thus, the guanidino benextramine analogs I [X = NC(NH2):NH] are selective, competitive antagonists of the postsynaptic NPY receptor in the femoral artery.
- IT 156272-83-2P 156272-84-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and neuropeptide Y antagonistic activity of)

RN 156272-83-2 CAPLUS

CN 1,6-Hexanediamine, N,N'-bis[6-[(2-naphthalenylmethyl)amino]-, tetrahydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

● 4 HCl

PAGE 1-B

RN 156272-84-3 CAPLUS

CN 1,6-Hexanediamine, N,N'-bis[6-[(2-naphthalenylmethyl)amino]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

- L15 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 1991:228377 CAPLUS
- DN 114:228377
- TI Preparation of polyazaalkenoic acids and analogs and their metal complexes for oxygen fixation
- IN Boisselier-Cocolios, Brigitte; Guilard, Roger; Jean, Christophe; Taurin, Laurent
- PA Air Liquide SA pour l'Etude et l'Exploitation des Procedes Georges Claude, Fr.
- SO PCT Int. Appl., 108 pp. CODEN: PIXXD2
- DT Patent
- LA French
- FAN.CNT 1

	PAT	CENT :	NO.			KIND DATE			APPLICATION NO.					DATE	
PI	WO	9009987 W: AU, CA, JP,			A1 US				WO 1990-FR124					19900222	
		•••	,	<b></b> /	,					FR	1989-2	2315		Α	19890222
	FR	2643	370			A1		1990	0824	FR	1989-2	2315			19890222
	FR	2643370				B1		1991	0823						
	CA	2027578			AA		1990	0823	CA	1990-2	20275	578		19900222	
										FR	1989-2	2315		Α	19890222
	AU	9051	759			A1		1990	0926	AU	1990-5	51759	€		19900222
	AU	6411	42			B2		1993	0916						
										FR	1989-2	2315			19890222
										WO	1990-F	R124	<del>l</del>	Α	19900222
	EΡ	3964	35			A1		1990	1107	EP	1990-4	10048	38		19900222
	EP	396435			B1	B1 19950621									
		R:	ΑT,	ΒE,	CH,	DE,	DK,	ES,	FR,	GB, GI	R, IT,	LI,	LU,	NL, S	Ξ
											1989-2				19890222
	ZA	9001	363			Α		1991	0327	ZA	1990-1	1363			19900222
											1989-2			Α	19890222
	JP	0350	4134			T2		1991	0912	_	1990-5		38		19900222
										FR	1989-2	2315		Α	19890222
										WO	1990-F	R124	l l	M	19900222
	US	6139	603			Α		2000	1031	US	1994-2	25323	33		19940602
										FR	1989-2	2315		Α	19890222

OS MARPAT 114:228377

AB The title compds., e.g., H[NH(CH2)2]4CO2H(I),

H2N(CH2)3NH(CH2)2N(CH2CO2H)CH2CH2NH2, whose metal complexes are useful for fixation of oxygen and thus for anal. of oxygen, etc., are prepared via, e.g., addition of a polyazaalkane to acrylonitrile followed by hydrolysis, N-alkylation of hexahydro-5H-1,4-diazepine-5-one with an aminoalkyl halide followed by hydrolysis. Acrylonitrile was added to triethylenetetramine over 30 min, the formed blue solution stirred at ambient temperature for 24 h, excess triethylenetetramine removed by distillation under reduced pressure, and the obtained nitrile hydrolyzed with H2SO4 to give I.  $Co(II) [PhCH2(NHCH2CH2)3CO2H] was obtained by dissolving PhCH2(NHCH2CH2)3CO2H.2H2SO4.H2O in water, adjusting the solution to pH 7.47 and then, at complete dissoln., to pH 2.25 followed by treatment with <math display="block">Co(OAc)2.4H2O. \quad Fixation of oxygen by the Co(II) [C6H5CH2(NHCH2CH2)3CO2H], obtained similarly, by forming the <math display="inline">\mu$ -peroxy complex LCoO2CoL (L = C6H5CH2(NHCH2)3CO2H) and recovering the oxygen by desorption is also

IT 133681-39-7P 133681-45-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of)

RN 133681-39-7 CAPLUS

demonstrated.

CN Propanenitrile, 3-[[2-[[2-[(2-naphthalenylmethyl)amino]ethyl]amino]ethyl]amino]- (9CI) (CA INDEX NAME)

RN 133681-45-5 CAPLUS

CN 2,5,8,11-Tetraazatetradecane-14-nitrile, 1-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

 $-CH_2-CN$ 

IT 133681-22-8P 133681-28-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, for complexing with metals for oxygen fixation)

RN 133681-22-8 CAPLUS

CN  $\beta$ -Alanine, N-[2-[[2-[(2-naphthalenylmethyl)amino]ethyl]amino]ethyl]-(9CI) (CA INDEX NAME)

RN 133681-28-4 CAPLUS

CN 2,5,8,11-Tetraazatetradecan-14-oic acid, 1-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

PAGE 1-B

— сн<sub>2</sub>— со<sub>2</sub>н

L15 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1990:514786 CAPLUS

DN 113:114786

TI [(1-Pyrenylmethyl)amino] alcohols, a new class of antitumor DNA intercalators. Discovery and initial amine side chain structure-activity studies:

AU Bair, Kenneth W.; Tuttle, Richard L.; Knick, Vincent C.; Cory, Michael; McKee, David D.

CS Div. Org. Chem., Burroughs Wellcome Co., Research Triangle Park, NC,

27709, USA

SO Journal of Medicinal Chemistry (1990), 33(9), 2385-93

CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

OS CASREACT 113:114786

The relationships among structure, interaction with DNA, and murine antitumor activity of a series of 1-pyrenylmethylamines were examined Binding studies show that all 1-pyrenylmethylamine derivs. bind to some extent to DNA by intercalation. The presence of addnl. basic amine groups in the side chain enhances DNA binding due to electrostatic interactions. Compds. containing only a single basic benzylic amine bind similarly to DNA. Only the presence of bulky side chains decreases the DNA interactions. Although antitumor activity is seen for (1-pyrenylmethyl)amino alcs., useful antitumor activity in the series is limited to congeners bearing the 2-amino-1,3-propanediol side chain. These derivs. bind moderately to DNA. DNA binding is a necessary but not sufficient criterion for antitumor activity. In addition, the strength of DNA binding does not correlate with the antitumor activity.

IT 127856-54-6P 127856-55-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation, DNA binding, and murine antitumor activity of)

RN 127856-54-6 CAPLUS

CN 1,3-Propanediamine, N-(3-aminopropyl)-N-methyl-N'-(1-pyrenylmethyl)-, trihydrochloride (9CI) (CA INDEX NAME)

$$Me$$
 $CH_2-NH-(CH_2)_3-N-(CH_2)_3-NH_2$ 

## ●3 HCl

RN 127856-55-7 CAPLUS

CN 1,3-Propanediamine, N-(3-aminopropyl)-N-methyl-N'-(1-pyrenylmethyl)- (9CI) (CA INDEX NAME)

$$Me$$
 $CH_2-NH-(CH_2)_3-N-(CH_2)_3-NH_2$ 

11 12 13 14 15 16 23 24 25 26 27 28 29 30 31 32 34 40 41 42 61 70 ring nodes : 1 2 3 4 5 6 7 18 19 20 21 22 46 47 48 49 50 51 52 8 9 10 17 55 56 57 63 64 65 66 67 68 chain bonds : 8-43 11-12 11-40 11-43 12-13 13-14 13-41 14-15 15-16 15-42 19-23 24-34 25-26 25-27 28-29 28-30 29-31 29-32 51-60 57-61 67-70 ring bonds : 6-10 7-8 8-9 9-10 17-18 17-22 18-19 19-20 1-2 1-6 2-3 3-4 4-5 5-6 5-7 48-49 49-50 50-51 52-53 52-57 53-54 54-55 55-56 20-21 21-22 46-47 46-51 47-48 63-68 64-65 65-66 66-67 67-68 56-57 63-64 exact/norm bonds : 11-40 13-41 15-16 15-42 24-34 25-26 25-27 28-29 28-30 51-60 57-61 67-70 exact bonds : 8-43 11-12 11-43 12-13 13-14 14-15 19-23 29-31 29-32 normalized bonds :  $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 5-7 \quad 6-10 \quad 7-8 \quad 8-9 \quad 9-10 \quad 17-18 \quad 17-22 \quad 18-19 \quad 19-20$ 48-49 49-50 50-51 52-53 52-57 53-54 54-55 55-56 20-21 21-22 46-47 46-51 47-48

G1:CH3,Et,i-Pr,n-Bu,t-Bu,n-Pr

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,t-Bu,[\*1],[\*2],[\*3],[\*4],[\*5],[\*6],[\*7]

56-57 63-64 63-68 64-65 65-66 66-67 67-68

Match level :

chain nodes :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom

34:Atom 40:CLASS 41:CLASS 42:CLASS 43:CLASS 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 55:Atom 57:Atom 60:Atom 61:Atom 63:Atom 66:Atom 67:Atom 68:Atom 70:Atom

11 12 13 14 15 16 23 24 25 26 27 28 29 30 31 32 34 40 41 42 43 60 61 70 ring nodes : 18 19 20 21 22 46 47 48 49 50 51 52 1 2 3 4 5 6 7 8 10 17 55 56 57 63 64 65 66 67 68 chain bonds : 8-43 11-12 11-40 11-43 12-13 13-14 13-41 14-15 15-16 15-42 19-23 24-34 25-26 25-27 28-29 28-30 29-31 29-32 51-60 57-61 67-70 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 17-18 17-22 18-19 19-20 48-49 49-50 50-51 52-53 52-57 53-54 54-55 55-56 20-21 21-22 46-47 46-51 47-48 66-67 67-68 56-57 63-64 63-68 64-65 65-66 exact/norm bonds : 25-26 25-27 28-29 28-30 51-60 57-61 67-70 11-40 13-41 15-16 15-42 24-34 exact bonds : 8-43 11-12 11-43 12-13 13-14 14-15 19-23 29-31 29-32 normalized bonds :  $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 5-7 \quad 6-10 \quad 7-8 \quad 8-9 \quad 9-10 \quad 17-18 \quad 17-22 \quad 18-19 \quad 19-20$ 20-21 21-22 46-47 46-51 47-48 48-49 49-50 50-51 52-53 52-57 53-54 54-55 55-56 56-57 63-64 63-68 64-65 65-66 66-67 67-68

G1:CH3,Et,i-Pr,n-Bu,t-Bu,n-Pr

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,t-Bu,[\*1],[\*2],[\*3],[\*4],[\*5],[\*6],[\*7]

Match level :

chain nodes :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom

34:Atom 40:CLASS 41:CLASS 42:CLASS 43:CLASS 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 60:Atom 61:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 70:Atom

chain nodes : 59 60 11 12 13 14 15 22 23 24 25 26 27 28 29 30 31 33 39 40 41 42 69 74 75 77 ring nodes : 5 6 7 9 10 16 17 18 19 20 21 45 46 47 48 49 50 8 54 55 56 62 63 64 65 66 67 chain bonds : 8-42 11-12 11-39 11-42 12-13 13-40 13-74 14-41 14-15 14-76 18-22 23-33 24-25 24-26 27-28 27-29 28-30 28-31 50-59 56-60 66-69 74-75 75-76 75-77 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19 19-20 20-21 45-46 45-50 46-47 47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55 55-56 62-63 62-67 63-64 64-65 65-66 66-67 exact/norm bonds : 11-39 13-40 14-41 14-15 23-33 24-25 24-26 27-28 27-29 50-59 56-60 66-69 75-77 exact bonds : 8-42 11-12 11-42 12-13 13-74 14-76 18-22 28-30 28-31 74-75 75-76 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19 19-20 20-21 45-46 45-50 46-47 47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55 55-56 62-63 62-67 63-64 64-65 65-66 66-67

G1:CH3,Et,i-Pr,n-Bu,t-Bu,n-Pr

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,t-Bu,[\*1],[\*2],[\*3],[\*4],[\*5],[\*6],[\*7]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 33:Atom

39:CLASS 40:CLASS 41:CLASS 42:CLASS 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 59:Atom 60:Atom 62:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 69:Atom 74:CLASS 75:CLASS 76:CLASS

69 72 73 74 75 ring nodes : 5 6 7 8 9 10 16 17 18 19 20 21 45 46 47 48 49 50 51 52 1 2 3 4 65 66 54 55 56 62 63 64 67 chain bonds : 8-42 11-12 11-39 11-42 12-13 13-40 13-72 14-41 14-15 14-74 18-22 23-33 24-25 24-26 27-28 27-29 28-30 28-31 50-59 56-60 66-69 72-73 73-74 73-75 ring bonds : 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19 1-2 1-6 2-3 3-4 4-5 5-6 5-7 48-49 49-50 51-52 51-56 52-53 53-54 54-55 19-20 20-21 45-46 45-50 46-47 47-48 62-67 63-64 64-65 65-66 55-56 62-63 exact/norm bonds : 11-39 13-40 14-41 14-15 23-33 24-25 24-26 27-28 27-29 50-59 56-60 66-69 73-75 exact bonds :

8-42 11-12 11-42 12-13 13-72 14-74 18-22 28-30 28-31 72-73 73-74 normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19 47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55 19-20 20-21 45-46 45-50 46-47 55-56 62-63 62-67 63-64 64-65 65-66 66-67

G1: CH3, Et, i-Pr, n-Bu, t-Bu, n-Pr

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,t-Bu,[\*1],[\*2],[\*3],[\*4],[\*5],[\*6],[\*7]

Match level :

11 12 13

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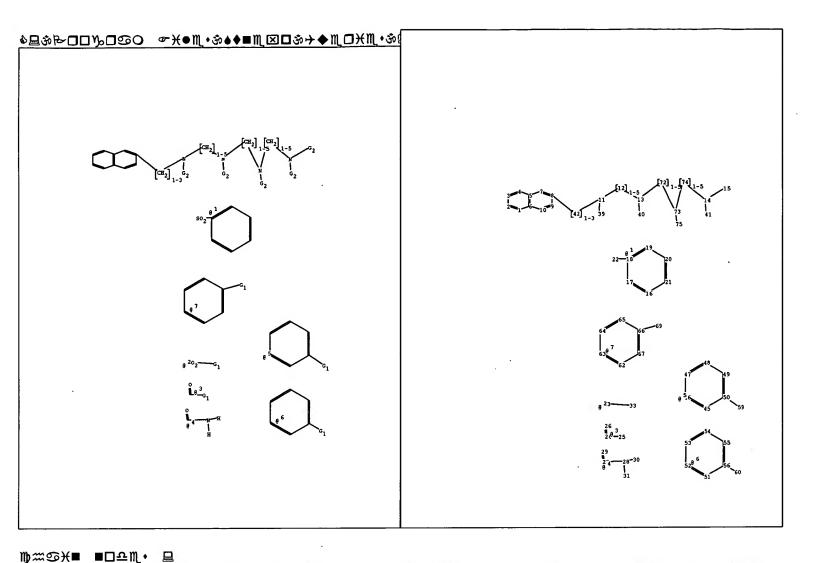
41

42

59

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 33:Atom

39:CLASS 40:CLASS 41:CLASS 42:CLASS 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 60:Atom 62:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 69:Atom 72:CLASS 73:CLASS 74:CLASS



8 **P** Bla v⊕ 20 \$ **₹**@ **6 €** 100 #100 **■**2€ □Ӿ≡⅓。 ■□≏♏∙  $\overline{C}$ Z 4 @ 1 2 TO **1** 9 20 12 90 20 20 21 20 100 22 200 സം∞െ∺െ പ്⊡∎≏• 🗟 820D20 2200210 **⊕**[10]**⊕**[ ପ∺≣%∘ ઈ□**≡**ဍ∙ 8002 800 **600**4 10 TO 1000 C تِوْلُونِ مِن اللهِ ا 10012 ○100° ○10° 8000B **###** 100 mu 20022 220026 2002**6** 20020 20028 88008 ₩⊠ॐ∰♦⋘■□□○ 원□■亞• 82022<u>—</u> **16** 2200210 ⊕ا∄اله ا സ്⊠ോത്♦ ପ୍⊡∎⊶ 🖻 10000 ■□□○ॐ●₭ж∭⊕ थि□■亞• 80D**é** 20000 <u>~</u>ø₽\$ 1000 8008 **€©** എന്നും 10000000 <u>~</u>300€ ~3000 # (C) (D) # 2 160 10010 100 EC 280088 22002 88008 280026 20028

6\*50 hm • m • m • ■ **□□8◆□○** ●四♥◆□○ ②□□●●□○ ◆B国● 20□♦§E@ ©10€8€□0 OD◆8BPC 戸歯型8◆□○ ●金目を◆□○ 10484□O Br@B& DO 22244□0 2**@**⊒8**♦**□○ 21@484□O e¶⊒4884 器画画覧◆□○ 

11 12 13 14 15 22 23 24 25 26 27 28 29 30 31 33 39 40 41 42 59 60 69 72 73 ring nodes : 9 10 16 17 18 19 20 21 45 46 47 48 49 50 1 2 3 4 5 6 7 8 54 55 56 62 63 64 65 66 67 chain bonds : 8-42 11-12 11-39 11-42 12-13 13-40 13-72 14-41 14-15 14-74 18-22 23-33 24-25 24-26 27-28 27-29 28-30 28-31 50-59 56-60 66-69 72-73 73-74 73-75 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19 47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55 19-20 20-21 45-46 45-50 46-47 62-63 62-67 63-64 64-65 65-66 exact/norm bonds : 11-39 13-40 14-41 14-15 23-33 24-25 24-26 27-28 27-29 50-59 56-60 66-69 73-75 exact bonds : 8-42 11-12 11-42 12-13 13-72 14-74 18-22 28-30 28-31 72-73 73-74 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19

19-20 20-21 45-46 45-50 46-47 47-48 48-49 49-50 51-52 51-56 52-53 53-54 54-55 55-56 62-63 62-67 63-64 64-65 65-66 66-67

G1: CH3, Et, i-Pr, n-Bu, t-Bu, n-Pr

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,t-Bu,[\*1],[\*2],[\*3],[\*4],[\*5],[\*6],[\*7]

## Match level :

chain nodes :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 33:Atom

39:CLASS 40:CLASS 41:CLASS 42:CLASS 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 60:Atom 62:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 69:Atom 72:CLASS 73:CLASS 74:CLASS 75:CLASS

67 70 71 72 73 ring nodes : 9 10 16 17 18 19 20 21 43 44 45 46 47 48 49 50 51 1 2 3 4 5 6 7 8 52 53 54 60 61 62 63 64 65 chain bonds : 8-42 11-12 11-39 11-42 12-13 13-40 13-70 14-41 14-15 14-72 18-22 23-33 24-25 24-26 27-28 27-29 28-30 28-31 48-57 54-58 64-67 70-71 71-72 71-73 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19 45-46 46-47 47-48 49-50 49-54 50-51 51-52 52-53 19-20 20-21 43-44 43-48 44-45 53-54 60-61 60-65 61-62 62-63 63-64 64-65 exact/norm bonds :  $11-39 \quad 13-40 \quad 14-41 \quad 14-15 \quad 23-33 \quad 24-25 \quad 24-26 \quad 27-28 \quad 27-29 \quad 48-57 \quad 54-58 \quad 64-67 \quad 71-73$ exact bonds : 8-42 11-12 11-42 12-13 13-70 14-72 18-22 28-30 28-31 70-71 71-72 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19 19-20 20-21 43-44 43-48 44-45 45-46 46-47 47-48 49-50 49-54 50-51 51-52 52-53 53-54 60-61 60-65 61-62 62-63 63-64 64-65

26 27 28 29

57 58

30 31 33 39 40 41 42

G1: CH3, Et, i-Pr, n-Bu, t-Bu, n-Pr

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,t-Bu,[\*1],[\*2],[\*3],[\*4],[\*5],[\*6],[\*7]

Match level : 1:Atom 2:

chain nodes :

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1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 33:Atom

39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 57:Atom 58:Atom 60:Atom 61:Atom 62:Atom 63:Atom 64:Atom 65:Atom 67:Atom 70:CLASS 71:CLASS 72:CLASS 73:CLASS

68 11 12 13 14 21 22 23 24 25 26 27 28 29 30 32 38 39 40 55 56 65 69 70 71 ring nodes : 9 10 15 16 17 18 19 20 41 42 43 44 45 46 47 5 6 7 1 2 3 4 - 8 50 51 52 58 59 60 61 62 63 chain bonds :  $8-40 \quad 11-12 \quad 11-38 \quad 11-40 \quad 12-13 \quad 13-39 \quad 13-68 \quad 14-70 \quad 17-21 \quad 22-32 \quad 23-24 \quad 23-25$ 26-28 27-29 27-30 46-55 52-56 62-65 68-69 69-70 69-71 ring bonds : 6-10 7-8 8-9 9-10 15-16 15-20 16-17 17-18 1-2 1-6 2-3 3-4 4-5 5-6 5-7 43-44 44-45 45-46 47-48 47-52 48-49 49-50 50-51 18-19 19-20 41-42 41-46 42-43 51-52 58-59 58-63 59-60 60-61 61-62 62-63 exact/norm bonds : 11-38 13-39 22-32 23-24 23-25 26-27 26-28 46-55 52-56 62-65 69-71 exact bonds : 8-40 11-12 11-40 12-13 13-68 14-70 17-21 27-29 27-30 68-69 69-70 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20 41-42 41-46 42-43 43-44 44-45 45-46 47-48 47-52 48-49 49-50 50-51

G1:CH3,Et,i-Pr,n-Bu,t-Bu,n-Pr

G2:H,CH3,Et,n-Pr,i-Pr,n-Bu,t-Bu,[\*1],[\*2],[\*3],[\*4],[\*5],[\*6],[\*7]

51-52 58-59 58-63 59-60 60-61 61-62 62-63

## Match level :

chain nodes :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 32:Atom 38:CLASS

39:CLASS 40:CLASS 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 55:Atom 56:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom 65:Atom 68:CLASS 69:CLASS 70:CLASS 71:CLASS